Abstract

Methods for searching stable docking models of biopolymer-ligand molecule complex, which comprise the steps of: (1) searching possible hydrogen-bond schemes between a biopolymer and a ligand molecule by preparing possible combination sets of hydrogen-bonding heteroatoms in the ligand molecule with dummy atoms located at the positions of heteroatoms that can be hydrogen-bond partners to hydrogen-bonding functional groups in the biopolymer; (2) estimating the possible the hydrogen-bond schemes between the biopolymer and ligand molecule and the possible conformations of a hydrogen-bonding part of the ligand molecule at the same time by comparing the distances between the dummy atoms with the distances between the hydrogen-bonding heteroatoms; and (3) obtaining the possible docking models of the biopolymer-ligand molecule complex by changing the coordinates of all atoms of the ligand molecule into the coordinate system of the biopolymer, according to the correspondences between the hydrogen-bonding heteroatoms in the ligand molecule and the dummy atoms in combination sets for each of the hydrogen-bond schemes and conformations obtained in the second step are provided.

According to the methods of the present invention, the structures of stable biopolymer-ligand molecule complex can be searched efficiently and precisely in a short time.